

Data dictionary for U.S.EPA ScienceHub dataset “*The Acute Toxicity of Major Ion Salts to Ceriodaphnia dubia: III. Mathematical Models for Mixture Toxicity*” (short name “MED Ion Tox Paper 3”). This dataset is contained in the zip file “MEDIonToxPaper3_Dataset.zip”, consisting of the following files:

I. 3 csv files named TDS-yy-nn.csv providing biological results and general chemistry for different experiments, with the following organization and format:

A. Each file describes a single experiment consisting of 2-6 tests regarding the acute toxicity of a single major ion salt or a complex ion mixture to *Ceriodaphnia dubia*.

B. Each file starts with several header rows with general experimental information.

C. Each file then has multiple blocks of information, each block providing data for one toxicity test.

D. Each block of information consists of 1-2 header rows with general test information, 2 rows of headings for data columns, 20 rows providing data for each test unit, and 2 blank rows separating it from the next block.

E. Each data row provides the following information for a test replicate:

1. The treatment identification as a percentage of the highest concentration
2. For single salt tests only, the nominal concentration (mg/L) of the salt
3. The initial number of test organisms
4. The number of surviving test organisms at 24 hours
5. The number of surviving test organisms at 48 hours
6. Hardness mg/L as CaCO₃. at test start
7. Alkalinity mg/L as CaCO₃. at test start
8. pH at test start
9. Dissolved Oxygen mg/L. at test start
10. Conductivity ms/cm. at test start
11. Dissolved Oxygen mg/L. at test end
12. Alkalinity mg/L as CaCO₃. at 24 hours
13. Alkalinity mg/L as CaCO₃, at 48 hours (test end)
14. pH at test end

15. Conductivity ms/cm. at test end
16. Temperature at test end

II. “*MEDIonToxPaper3_Supplement3Final*” in .xlsx, .csv, and .pdf formats providing the following information regarding each toxicity test from the above toxicity test protocols, with a caption providing other information regarding the information

1. Test ID
2. pH at LC50
3. Total Na Concentration (mM) at LC50
4. Total K Concentration (mM) at LC50
5. Total Ca Concentration (mM) at LC50
6. Total Mg Concentration (mM) at LC50
7. Total Cl Concentration (mM) at LC50
8. Total SO₄ Concentration (mM) at LC50
9. Alkalinity (meq/L) at LC50
10. Ca⁺² Activity (mM) at LC50
11. Mg⁺² Activity (mM) at LC50
12. Na⁺¹ Activity (mM) at LC50
13. K⁺¹ Activity (mM) at LC50
14. Cl⁻¹ Activity (mM) at LC50
15. SO₄⁻² Activity (mM) at LC50
16. CO₃⁻² Activity (mM) at LC50
17. HCO₃⁻¹ Activity (mM) at LC50
18. H₂CO₃* Activity (mM) at LC50
19. Nominal Osmolarity (mOsm/L) at LC50
20. Calculated Osmolarity (mOsm/L) at LC50

III. “*MEDIonToxPaper3_Supplement1Final*” in .xlsx, .csv, and .pdf formats providing the following information regarding data used in development of the general ion toxicity models.

1. Test ID
 - For single chemical tests:
 2. Chemical name
 3. Culture water

4. Dilution water
- For binary mixture tests:
2. Chemical A name
3. Chemical B name
4. Mixture description
5. Calcium Activity (mM) at LC50
6. Osmolarity (mOsm/L) at LC50
7. Total Ca Concentration (mM) at LC50
8. Nominal Osmolarity (mOsm/L) at LC50

IV. “*MEDIonToxPaper3_Supplement2Final*” in .xlsx, .csv, and .pdf formats providing the following information regarding data used in development of the Mg/Ca toxicity models.

1. Test ID
- For single chemical tests:
2. Chemical name
3. Culture water
4. Dilution water
- For binary mixture tests:
2. Chemical A name
3. Chemical B name
4. Mixture description
5. Calcium Activity (mM) at LC50
6. Magnesium Activity (mM) at LC50
7. Total Ca Concentration (mM) at LC50
8. Magnesium Concentration (mM) at LC50